

REPORT DOCUMENTATION PAGE

*Form Approved
OMB No. 0704-0188*

Public reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing this collection of information. Send comments regarding this burden estimate or any other aspect of this collection of information, including suggestions for reducing this burden to Department of Defense, Washington Headquarters Services, Directorate for Information Operations and Reports (0704-0188), 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302. Respondents should be aware that notwithstanding any other provision of law, no person shall be subject to any penalty for failing to comply with a collection of information if it does not display a currently valid OMB control number. **PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ADDRESS.**

1. REPORT DATE (DD-MM-YYYY) 22 June 2015		2. REPORT TYPE Briefing Charts		3. DATES COVERED (From - To) 19 June 2015 – 22 June 2015	
4. TITLE AND SUBTITLE Optimal Runge-Kutta Schemes for High-order Spatial and Temporal Discretizations		5a. CONTRACT NUMBER			
		5b. GRANT NUMBER			
		5c. PROGRAM ELEMENT NUMBER Q12J			
6. AUTHOR(S) Mundis, N., Edoh, A. and Sankaran, V.		5d. PROJECT NUMBER			
		5e. TASK NUMBER			
		5f. WORK UNIT NUMBER Q12J			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQR 5 Pollux Drive Edwards AFB, CA 93524-7048		8. PERFORMING ORGANIZATION REPORT NO.			
9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory (AFMC) AFRL/RQR 5 Pollux Drive Edwards AFB, CA 93524-7048		10. SPONSOR/MONITOR'S ACRONYM(S)			
		11. SPONSOR/MONITOR'S REPORT NUMBER(S) AFRL-RQ-ED-VG-2015-268			
12. DISTRIBUTION / AVAILABILITY STATEMENT Approved for public release; distribution unlimited					
13. SUPPLEMENTARY NOTES For presentation at 22nd AIAA Computational Fluid Dynamics Conference; Dallas, TX; 22 June 2015 PA Case Number: #15352; Clearance Date: 6/29/2015					
14. ABSTRACT Viewgraphs/Briefing Charts					
15. SUBJECT TERMS N/A					
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	18. NUMBER OF PAGES 29	19a. NAME OF RESPONSIBLE PERSON V. Sankaran
a. REPORT Unclassified	b. ABSTRACT Unclassified	c. THIS PAGE Unclassified			19b. TELEPHONE NO (include area code) N/A



Optimal Runge-Kutta Schemes for High-order Spatial and Temporal Discretizations

Nathan L. Mundis – ERC, Inc.
Ayaboe K. Edoh – UCLA
Venke Sankaran – AFRL/RQ



2015 AIAA SciTech
June 23, 2015

Outline



- **Introduction**
- **Governing Equations**
 - Spatial Discretizations
 - Temporal Discretizations
- **Von Neumann Analysis (VNA)**
- **Computational Results**
 - One-dimensional Wave
 - Three-dimensional Vortex
- **Conclusions and Future Work**

Introduction

- High-order in space is now commonplace
- High-order in time... not so much...
- Is this sufficient? Is high-order in time needed?
- Limiting Fact: There are no A-stable backward-difference formula (BDF) methods with $> 2^{nd}$ -order accuracy
- Thus, multistage methods, like Runge-Kutta (RK) methods, must be used for 3^{rd} - and higher-order
- Explicit RK methods are not amenable to stiff problems

Objective: To find optimal diagonally-implicit Runge-Kutta time integrators for use with high-order spatial discretizations





Governing Equations

- **Dual Time Stepping:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}_i}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H}$$

$$\mathbf{F}_i = [\rho u_i \quad \rho u_i u_j + p \delta_{ij} \quad u_i \rho h_0]^T \text{ where } h_0 = e_0 + \frac{p}{\rho}$$

- **Quasi-Linear Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \underline{\Lambda} \frac{\partial \mathbf{Q}}{\partial x_i} = \frac{\partial \mathbf{V}_i}{\partial x_i} + \mathbf{H}$$

$$\underline{\Lambda} = diag \{u_i + c, u_i, u_i - c\}$$

- **Residual Form:**

$$\frac{\partial \mathbf{Q}}{\partial \tau} + \frac{\partial \mathbf{Q}}{\partial t} + \mathbf{R}_s(\mathbf{Q}) = 0 \quad where \quad \mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$



Spatial Discretizations

- Central Differences with added artificial dissipation

- Central differences:

$$\frac{\partial \Upsilon_j}{\partial x_i} \Big|_{II} = \frac{\Upsilon_{j+1} - \Upsilon_{j-1}}{2\Delta x_i}$$

$$\frac{\partial \Upsilon_j}{\partial x_i} \Big|_{IV} = \frac{-\Upsilon_{j+2} + 8\Upsilon_{j+1} - 8\Upsilon_{j-1} + \Upsilon_{j-2}}{12\Delta x_i}$$

$$\frac{\partial \Upsilon_j}{\partial x_i} \Big|_{VI} = \frac{\Upsilon_{j+3} - 9\Upsilon_{j+2} + 45\Upsilon_{j+1} - 45\Upsilon_{j-1} + 9\Upsilon_{j-2} - \Upsilon_{j-3}}{60\Delta x_i}$$

where Υ could be \mathbf{F}_i or \mathbf{Q} depending on the form of the equations

- Scalar artificial dissipation:

$$\mathbf{R}_s = \frac{\partial \mathbf{F}_i}{\partial x_i} - \varepsilon_\eta \parallel \lambda \parallel \frac{\partial^\eta \mathbf{Q}}{\partial x_i^\eta} - \frac{\partial \mathbf{V}_i}{\partial x_i} - \mathbf{H}$$

where η is even and one more than the order of accuracy

$$\parallel \lambda \parallel = |u_i| + c \quad \varepsilon_{II} = \frac{\Delta x_i}{2}, \quad \varepsilon_{IV} = -\frac{\Delta x_i^3}{12}, \quad \varepsilon_{VI} = \frac{\Delta x_i^5}{60}.$$



Temporal Discretizations



- Runge-Kutta Methods:

$$\begin{array}{c|ccccc} & a_{11} & a_{12} & a_{13} & \cdots & a_{1s} \\ c_1 & & & & & \\ c_2 & a_{21} & a_{22} & a_{23} & \cdots & a_{2s} \\ c_3 & a_{31} & a_{32} & a_{33} & \cdots & a_{3s} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ c_{s-1} & a_{(s-1)1} & a_{(s-1)2} & a_{(s-1)3} & \cdots & a_{(s-1)s} \\ c_s & a_{s1} & a_{s2} & a_s 3 & \cdots & a_{ss} \\ \hline & b_1 & b_2 & b_3 & \cdots & b_s \\ & \hat{b}_1 & \hat{b}_2 & \hat{b}_3 & \cdots & \hat{b}_s \end{array}$$

$$t^k = t^n + c_k \Delta t \quad \mathbf{Q}^k = \mathbf{Q}^n - \Delta t \sum_{j=1}^s a_{kj} \mathbf{R}_s^j(\mathbf{Q}^j) \quad k = 1, 2, \dots, s$$

$$\mathbf{Q}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^s b_j \mathbf{R}_s^j(\mathbf{Q}^j) \quad \hat{\mathbf{Q}}^{n+1} = \mathbf{Q}^n - \Delta t \sum_{j=1}^s \hat{b}_j \mathbf{R}_s^j(\mathbf{Q}^j)$$

$$\epsilon^{n+1} = \mathbf{Q}^{n+1} - \hat{\mathbf{Q}}^{n+1}$$



ESDIRK Methods



- **Explicit first stage Singly-Diagonally
Implicit Runge-Kutta**

- Stiffly accurate

- Second-order stage accuracy

- FSAL – First is the Same As Last

$c_1 = 0$	0	0	0	0	...	0	0
c_2		a_{21}	λ	0	...	0	0
c_3		a_{31}	a_{32}	λ	...	0	0
:	:	:	:	:	...	:	:
c_{s-1}	$a_{(s-1)1}$	$a_{(s-1)2}$	$a_{(s-1)3}$...	λ	0	
$c_s = 1$	b_1	b_2	b_3	...	b_{s-1}	λ	
	\hat{b}_1	\hat{b}_2	\hat{b}_3	...	\hat{b}_{s-1}	\hat{b}_s	



ESDIRK3 and 4



	0	0	0	0
$\frac{1767732205903}{2027836641118}$	$\frac{1767732205903}{4055673282236}$	$\frac{1767732205903}{4055673282236}$	0	0
$\frac{3}{5}$	$\frac{2746238789719}{10658868560708}$	$-\frac{640167445237}{6845629431997}$	$\frac{1767732205903}{4055673282236}$	0
1	$\frac{1471266399579}{7840856788654}$	$-\frac{4482444167858}{7529755066697}$	$\frac{11266239266428}{11593286722821}$	$\frac{1767732205903}{4055673282236}$
	$\frac{1471266399579}{7840856788654}$	$-\frac{4482444167858}{7529755066697}$	$\frac{11266239266428}{11593286722821}$	$\frac{1767732205903}{4055673282236}$

Implicit, Third-order ESDIRK3

	0	0	0	0
$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{4}$	0	0
$\frac{83}{250}$	$-\frac{1743}{31250}$	$-\frac{1}{4}$	0	0
$\frac{31}{50}$	$-\frac{654441}{2922500}$	$\frac{174375}{388108}$	$\frac{1}{4}$	0
$\frac{17}{20}$	$-\frac{71443401}{120774400}$	$\frac{730878875}{902184768}$	$\frac{2285395}{8070912}$	$\frac{1}{4}$
1	0	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$-\frac{2260}{8211}$
	$\frac{82889}{524892}$	$\frac{15625}{83664}$	$\frac{69875}{102672}$	$-\frac{2260}{8211}$

Implicit, Fourth-order ESDIRK4

Distribution A – Approved for public release; Distribution Unlimited



ESDIRK5

The single biggest drawback of using these schemes is typing them out!

Distribution A = Approved for public release: Distribution Unlimited



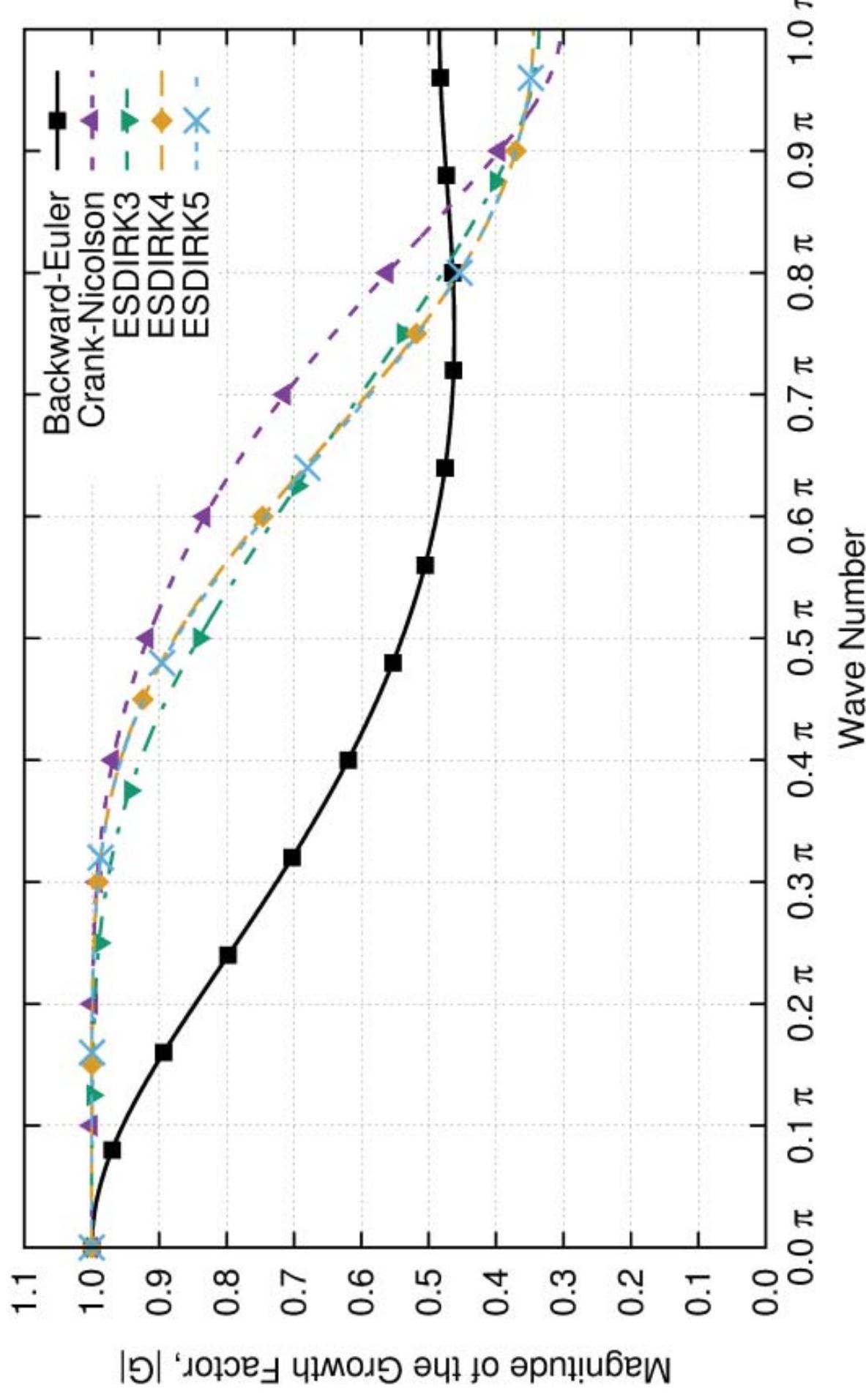
Von Neumann Analysis

- Often used to study stability of schemes
- Von Neumann analysis is used to compare schemes for accuracy
 - Dissipation error
 - Dispersion error
- Assumes linear, periodic problems
- VNA theory and more results are in the associated paper



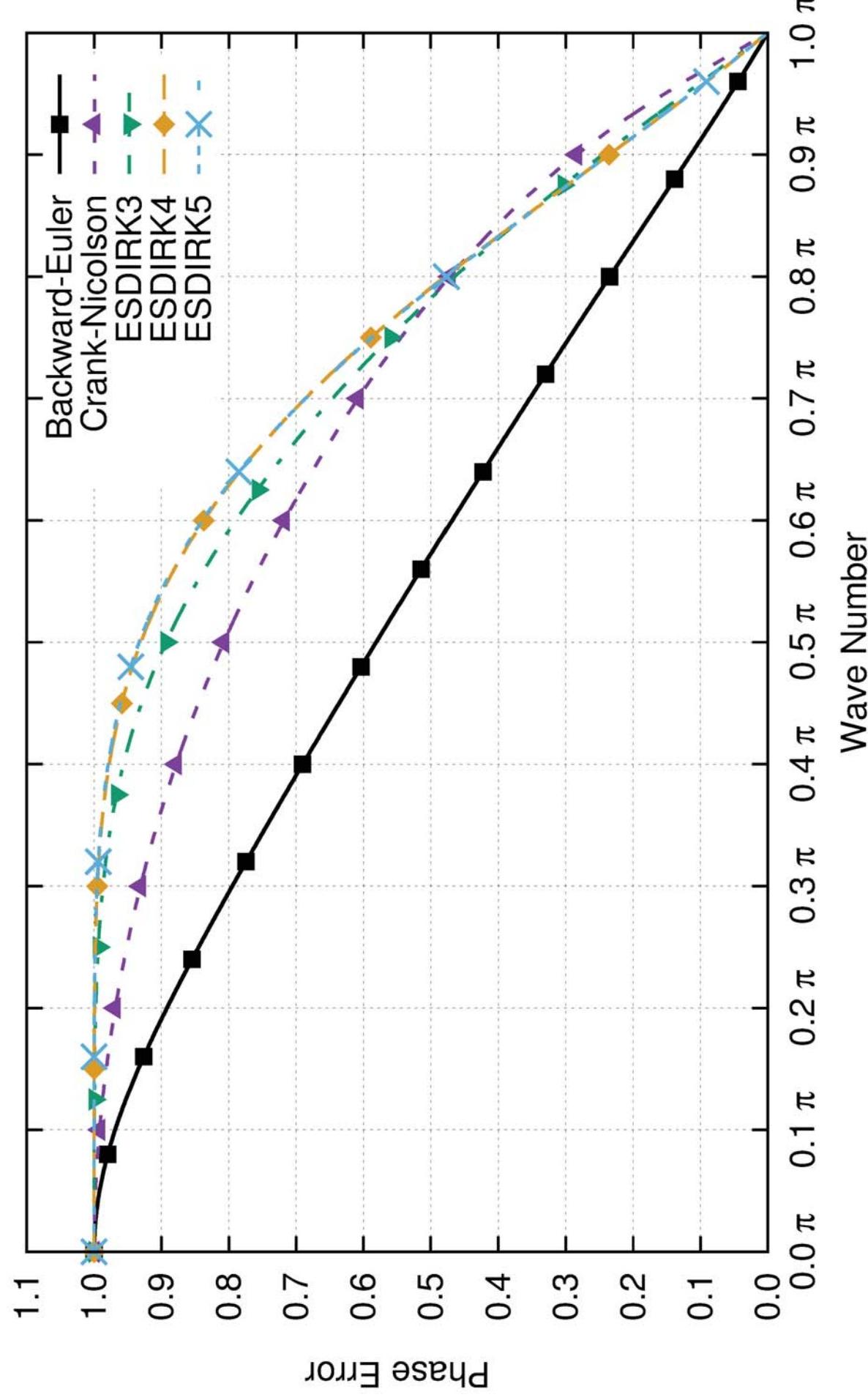


Dissipation, $CFL = 1.0$



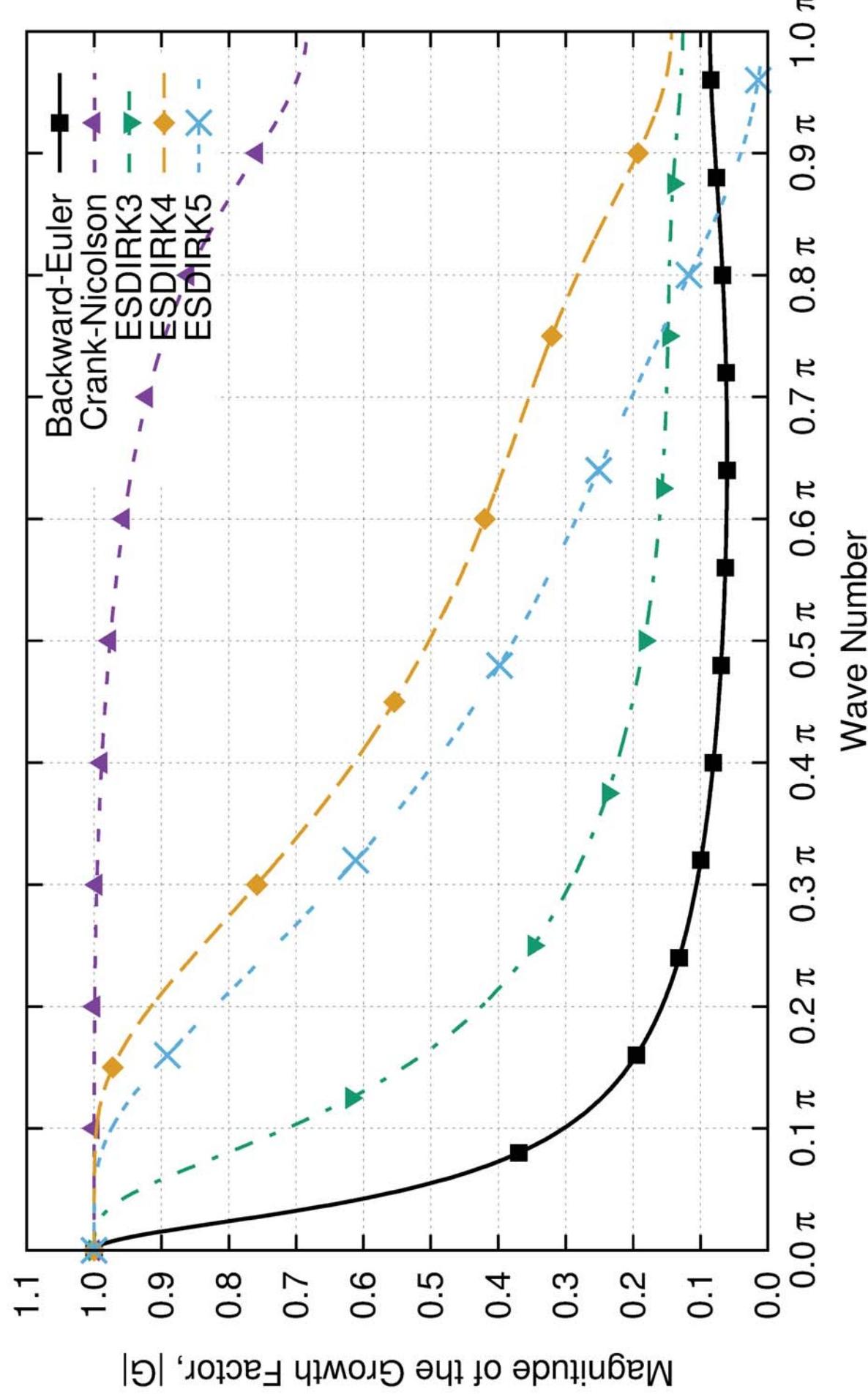


Dispersion, $CFL = 1.0$



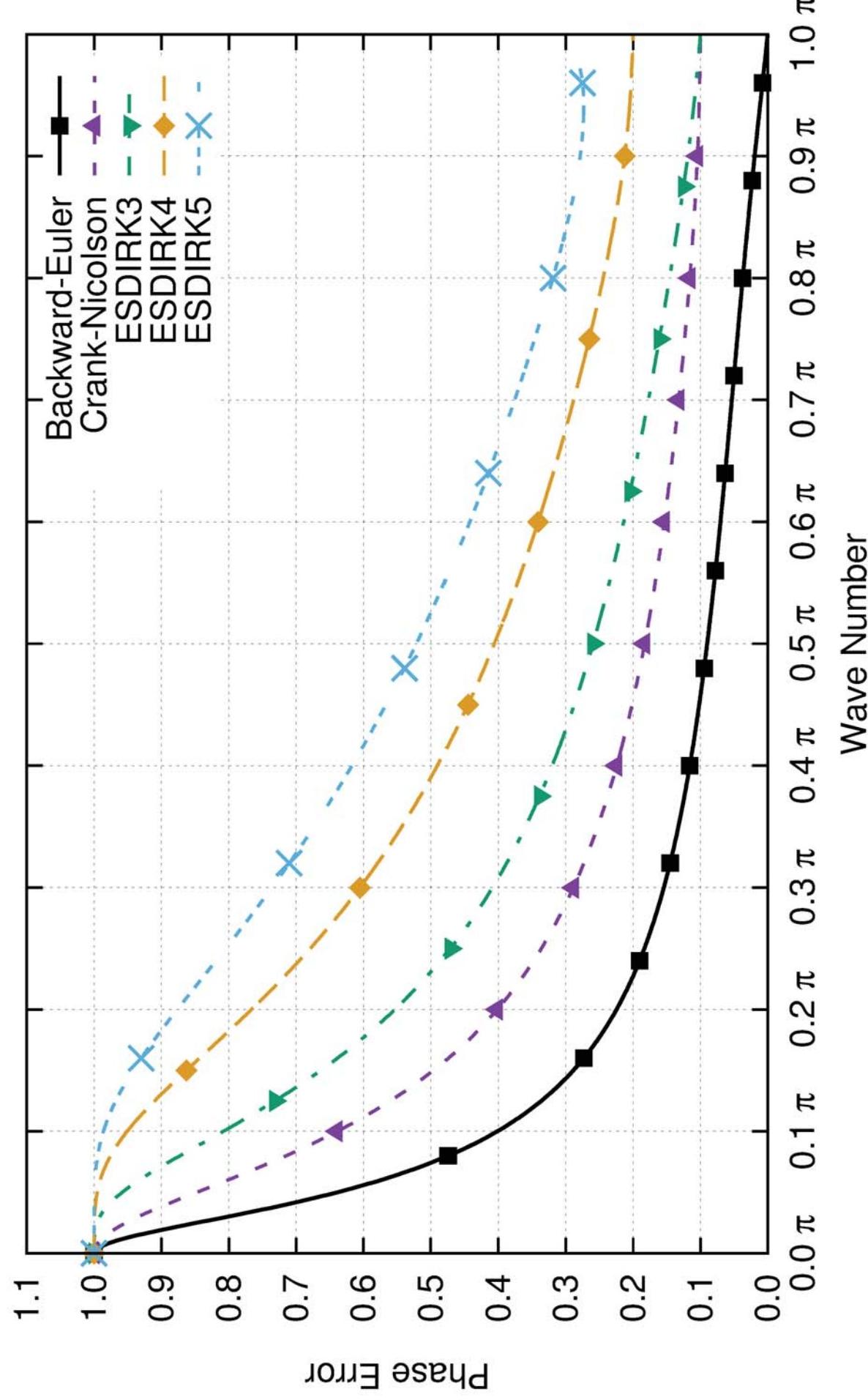


Dissipation, $CFL = 10.0$





Dispersion, $CFL = 10.0$





1-D Acoustic Wave

- Unperturbed Mach number of 0.5

$$\rho_\infty = 8.7077 \times 10^{-1} \frac{kg}{m^3}$$

$$\rho u_\infty = 1.7458 \times 10^2 \frac{kg}{m^2 \cdot s}$$

$$T_\infty = 400 K$$

$$R_\infty = 2.871 \times 10^2 \frac{J}{kg \cdot K}$$

$$\gamma = 1.4$$

- Perturbation wave - 20 points per wave resolution

$$\begin{aligned} Q_o &= Q_\infty + M \delta \hat{Q}_{u,u \pm c} \\ \delta \hat{Q}_{u,u \pm c} &= \hat{\delta} \cdot \cos(kx) \end{aligned}$$

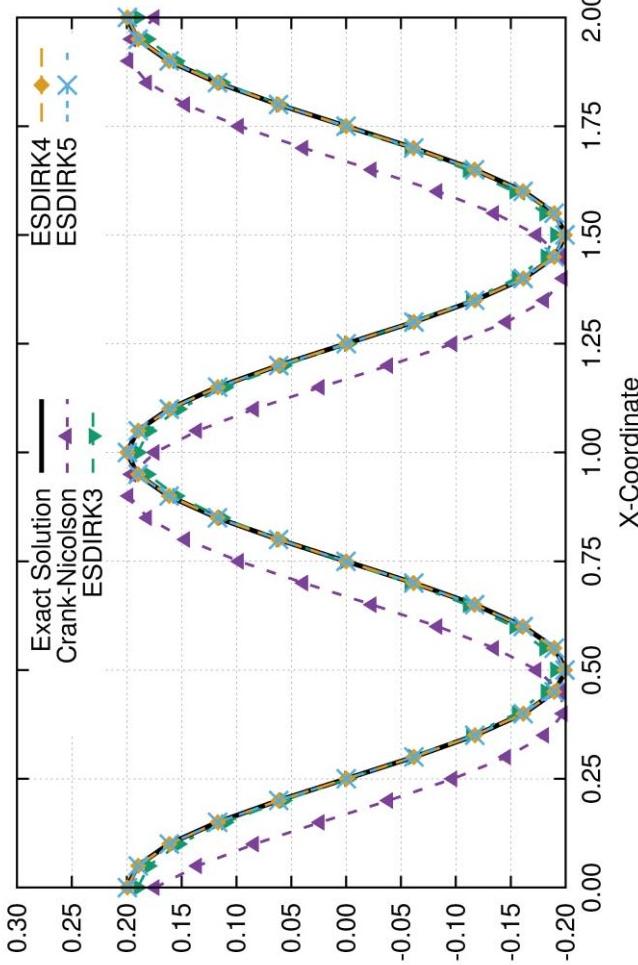
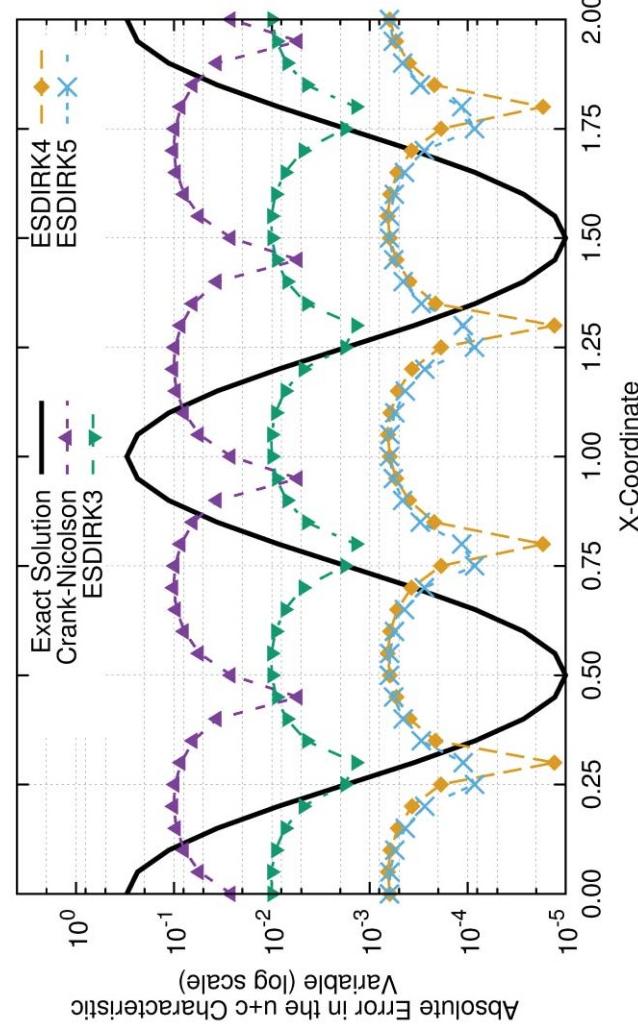
where $\hat{\delta} = 0.01$

- More results in the paper

1-D, $CFL = 1.0$, 10 Periods



Scheme	Dissipation Error		Dispersion Error	
	VNA	Simulation	VNA	Simulation
Crank-Nicolson	3.05×10^{-3}	1.00×10^{-2}	8.11×10^{-2}	8.11×10^{-2}
ESDIRK3	5.02×10^{-2}	5.02×10^{-2}	1.51×10^{-3}	1.53×10^{-3}
ESDIRK4	3.13×10^{-3}	3.13×10^{-3}	1.50×10^{-4}	1.58×10^{-4}
ESDIRK5	3.14×10^{-3}	3.14×10^{-3}	6.78×10^{-5}	6.90×10^{-5}

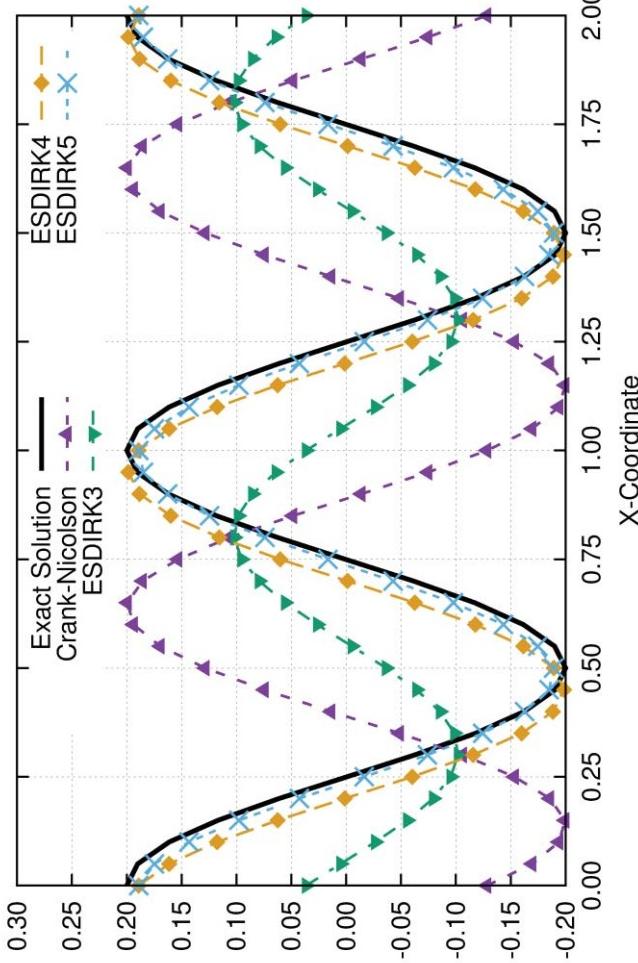
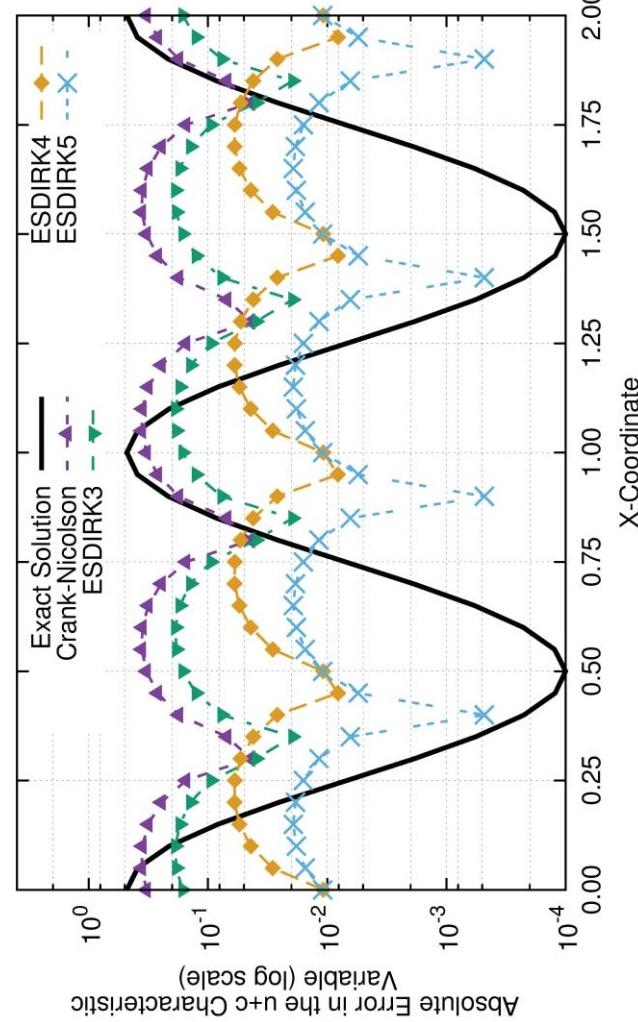




1-D, CFL = 10.0, 1 Period



Scheme	Dissipation Error		Dispersion Error	
	VNA	Simulation	VNA	Simulation
Crank-Nicolson	9.02×10^{-5}	2.44×10^{-3}	3.61×10^{-1}	3.61×10^{-1}
ESDIRK3	4.99×10^{-1}	4.90×10^{-1}	1.92×10^{-1}	1.92×10^{-1}
ESDIRK4	7.22×10^{-3}	7.25×10^{-3}	4.90×10^{-2}	4.90×10^{-2}
ESDIRK5	5.10×10^{-2}	5.46×10^{-2}	1.38×10^{-2}	1.39×10^{-2}

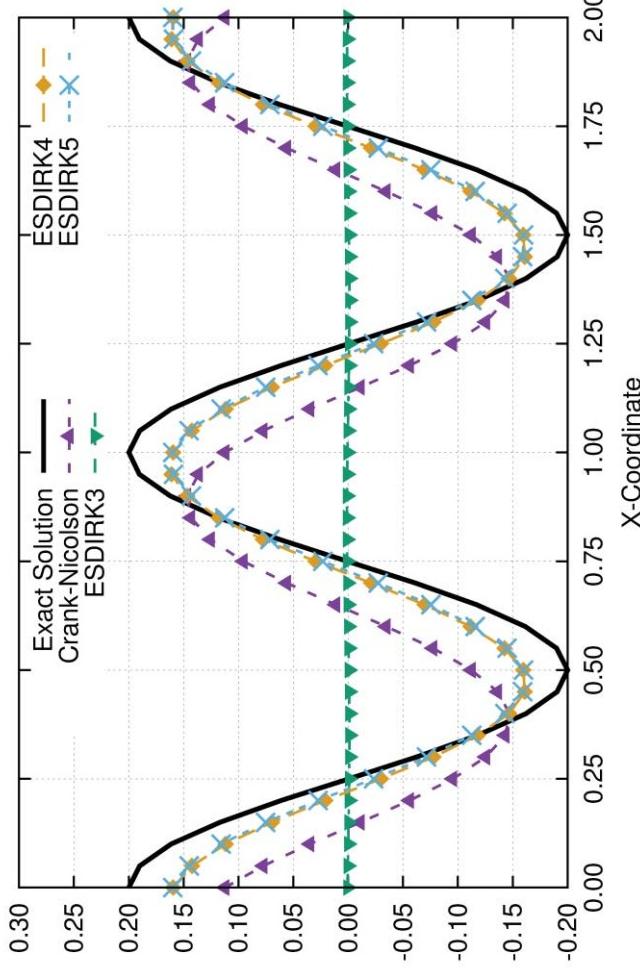
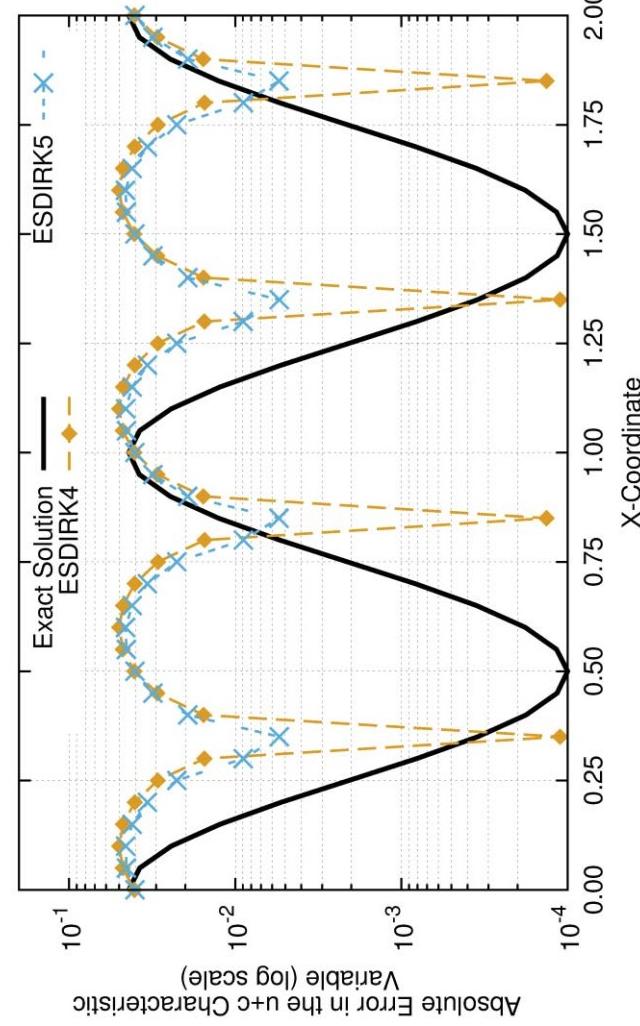




1-D, $CFL = 1.0, 1000$ Periods



Scheme	VNA	Dissipation Error	Dispersion Error
Crank-Nicolson	2.63×10^{-1}	2.65×10^{-1}	8.11×10^0
ESDIRK3	9.94×10^{-1}	9.94×10^{-1}	1.51×10^{-1}
ESDIRK4	2.69×10^{-1}	1.95×10^{-1}	1.50×10^{-2}
ESDIRK5	2.70×10^{-1}	2.01×10^{-1}	6.78×10^{-3}





3-D Isentropic Vortex



- Free-stream Mach number of 0.5

$$\rho_\infty = 1.0 \frac{kg}{m^3}, \quad \rho u_\infty = 200.0 \frac{kg}{m^2.s}, \quad \rho v_\infty = 0.0 \frac{kg}{m^2.s}, \quad \rho w_\infty = 0.0 \frac{kg}{m^2.s}, \quad \rho e_{0,\infty} = 305714.3 \frac{kg}{m.s^2}$$

$$R_\infty = 287.11 \frac{J}{kg.K} \text{ and } \gamma = 1.4$$

- Perturbation - 11 points across the vortex

$$\delta u = -\sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (y - y_0) e^{\phi(1-r^2)}$$

$$\delta v = \sqrt{R_\infty T_\infty} \frac{\alpha}{2\pi} (x - x_0) e^{\phi(1-r^2)}$$

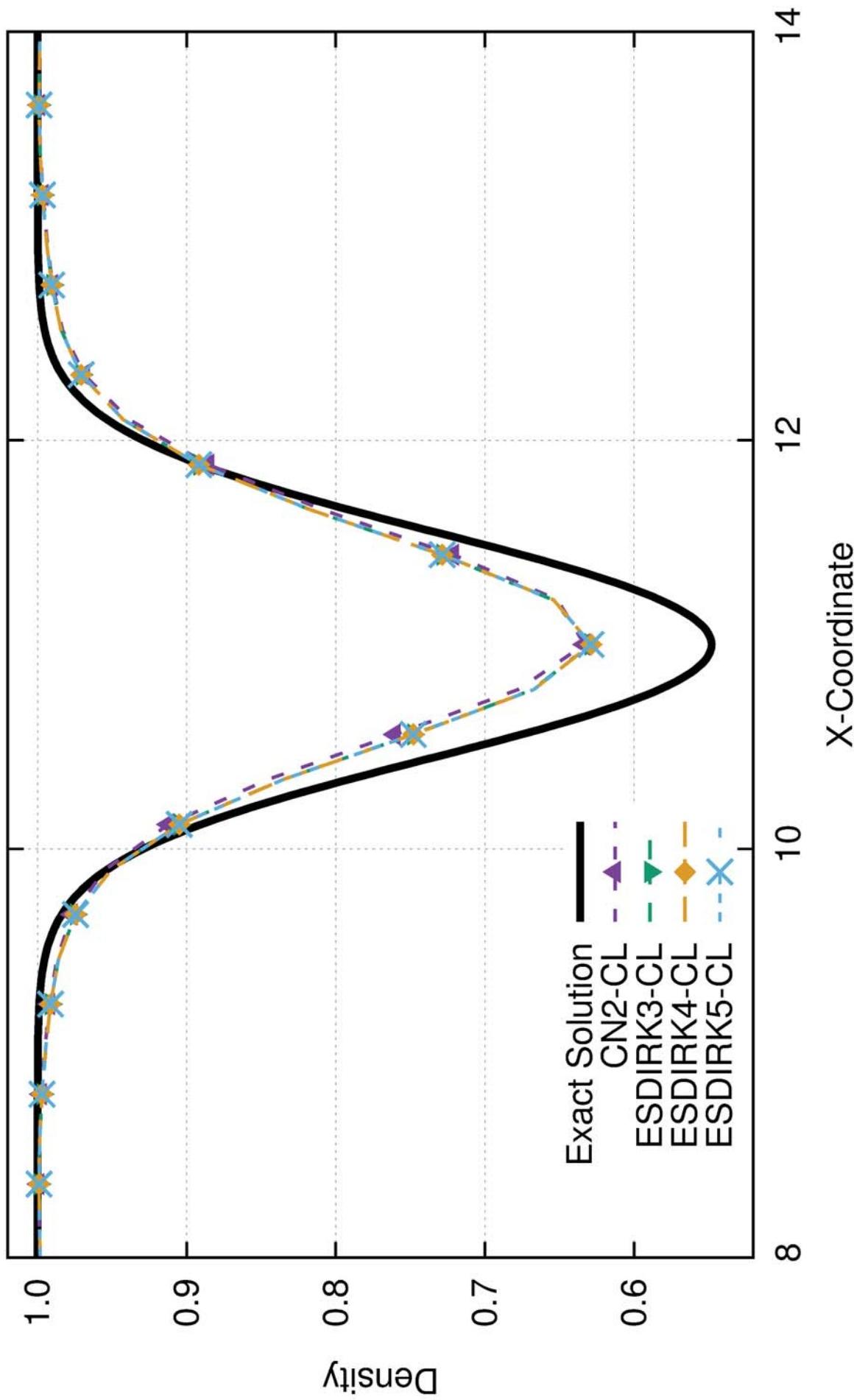
$$\delta T = T_\infty \frac{\alpha^2 (\gamma - 1)}{16 \phi \gamma \pi^2} e^{2\phi(1-r^2)}$$



- More results in the paper

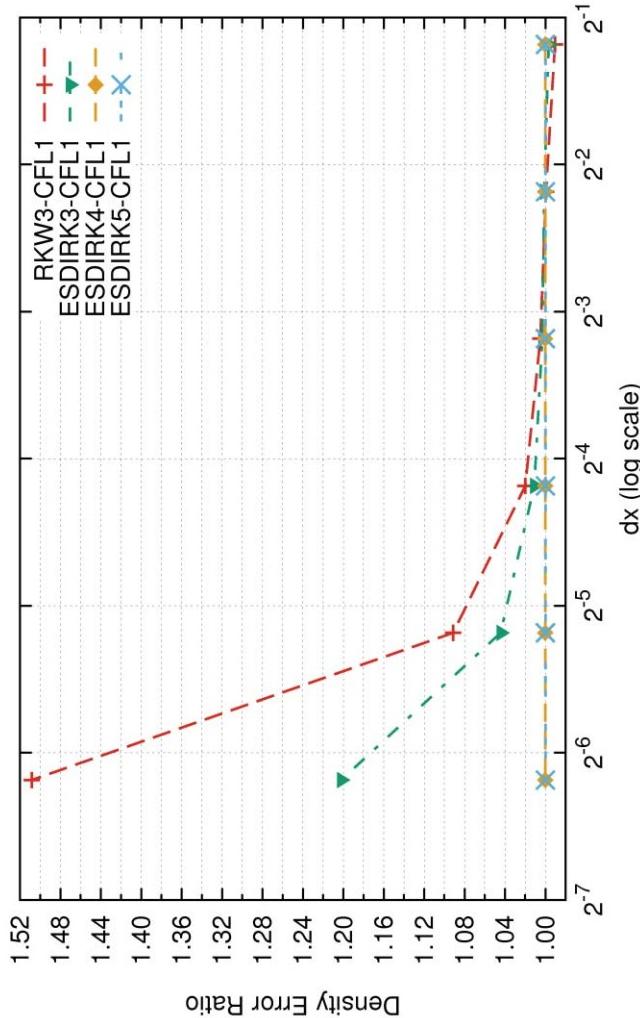
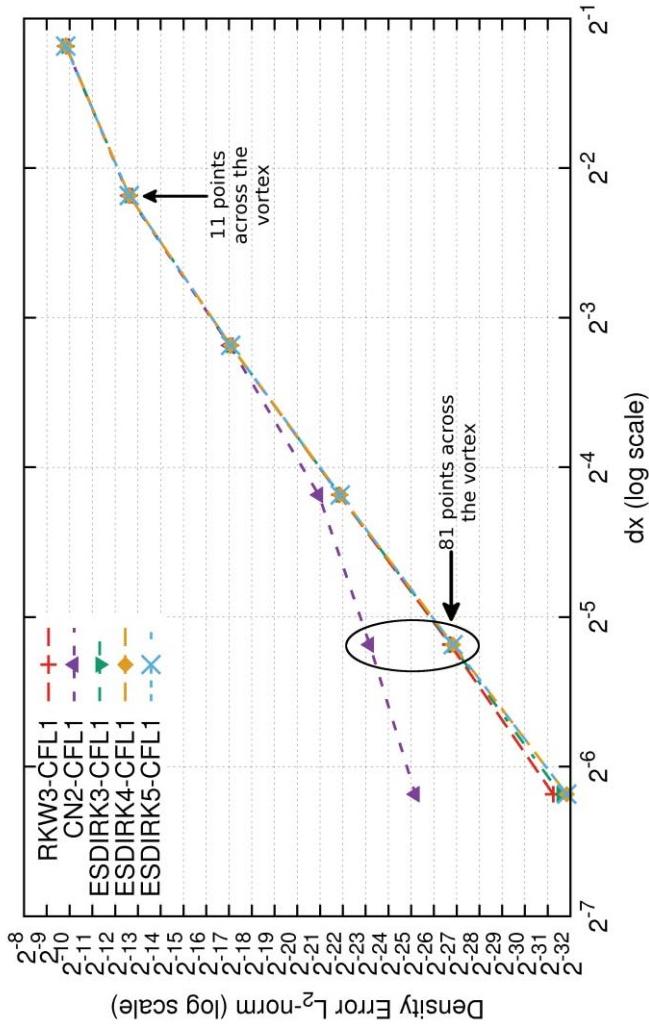


3-D, $CFL = 1.0$, 40 Lengths, 11 Points Across the Vortex



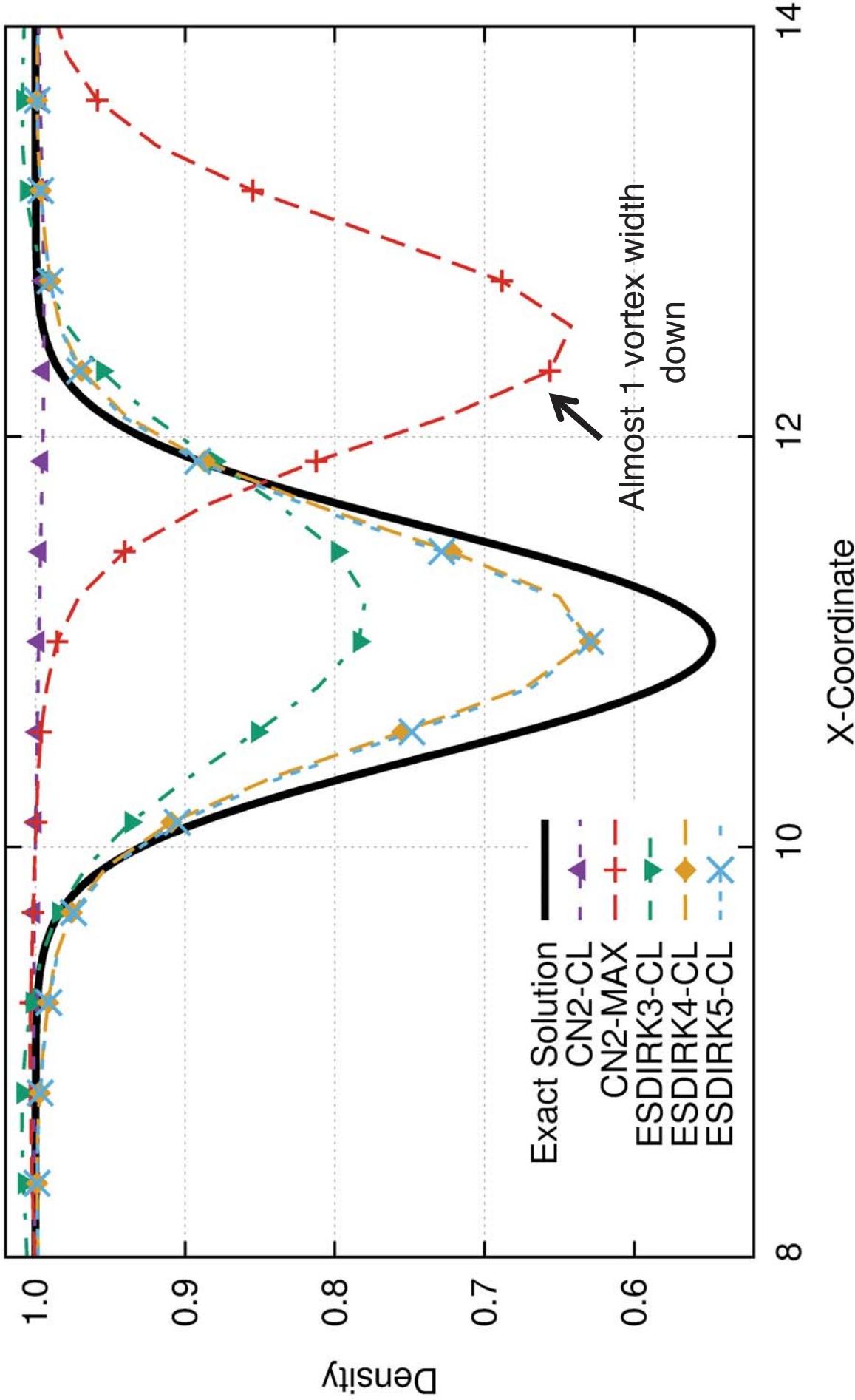


3-D, $CFL = 1.0$ Different Resolutions





3-D, $CFL = 8.0$, 40 Lengths, 11 Points Across the Vortex

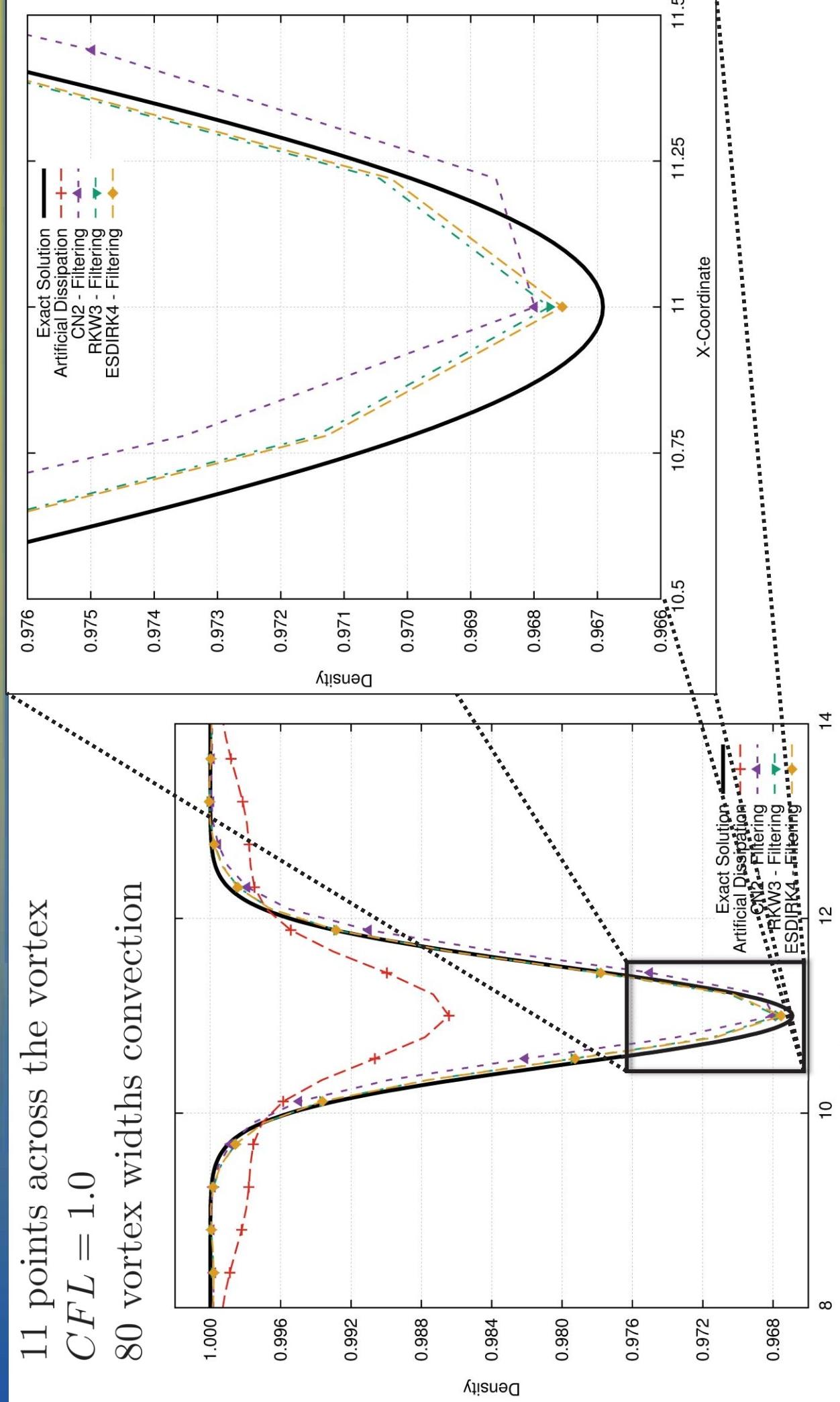




Sneak Peak: Filtering



11 points across the vortex
 $CFL = 1.0$
80 vortex widths convection



Conclusions



- **2nd- and 3rd-order time integrators for 5th-order spatial schemes are inadequate**
 - The same order of spatial and temporal discretizations is preferable
 - However, ESDIRK5 is not much better than ESDIRK4
 - 7 implicit stages vs. 5 implicit stages
- **Higher-order time integrators:**
 - Do not show significant improvement on coarse grids at CFL of one
 - Are better at high CFL number
 - Are better on highly refined grids
- **Spatial error usually dominates for typical CFL numbers and grid resolutions**
 - Central difference plus artificial dissipation schemes are inadequate

Future Work



- Implement more accurate spatial schemes of the same orders of accuracy
 - Compact-difference schemes
 - Filtering schemes
- Derive better ESDIRK schemes tailored to the desired dissipation and dispersion properties
- Add preconditioning to take maximum advantage of the ESDIRK time integrators for stiff problems
 - Improved convergence efficiency
 - Improved solution accuracy

Questions????





Extra Slides





3-D, $CFL = 8.0$ Different Resolutions

